Thermodynamics of 1-flavor QCD [*]

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We present first results, for heavy to moderate quark masses, of a study of thermodynamic properties of 1-flavor QCD, using the multiboson algorithm.

1. Introduction

Our understanding of QCD thermodynamics is still very incomplete. Simulations of the 0-flavor (quenched) lattice theory are just starting to produce results in line with continuum expectations. The situation in the 2- and 3-flavor cases is still rather murky (for an excellent review, see [1], or this volume). Additional information for different numbers n_f of quark flavors is clearly desirable to build a coherent picture such as proposed in [2] near the chiral limit. The study of QCD with exotic n_f has focused on many flavors [3]. Perhaps because of algorithmic difficulties, 1-flavor QCD has been largely ignored, although it has particularly interesting properties.

It is impossible to make a $\pi - \sigma$ doublet with only 1 quark species, so there is no chiral symmetry to speak of at vanishing quark mass. The low-lying meson spectrum consists of the "f_0" ($\overline{q}q$) and the "η'" ($\overline{q}\gamma_5 q$). The η' correlator $G_{\eta'}(x,y) = |D^{-1}(x,y)|^2 - D^{-1}(x,x)D^{-1}(y,y)$ contains 2 pieces, only the first of which, analogous to the pion correlator, becomes massless (constant) at $m_q = 0$. Thus the chiral phase transition and the associated Goldstone boson are absent in the 1-flavor theory [2]. In the heavy quark regime, on the other hand, the effect of dynamical quarks is still analogous to that of an external magnetic field on the equivalent Potts system.

Just like in the 2-flavor case, this external field weakens the phase transition, possibly turning it into a crossover. Thus, as the quark mass is decreased, one might expect the first-order deconfinement transition to become second-order, with an end-point at some finite quark mass. For any lighter quark, only a crossover would be seen.

Of course, testing this scenario requires careful finite-size scaling studies. As a first step, we present here preliminary results obtained on an $8^3 \times 4$ lattice. We use Wilson fermions, and try to follow the critical line in the (κ, β) plane, starting from $\kappa = 0$.

2. Algorithm

The standard algorithm to study any number of flavors is the R-algorithm [4], where the effect of the fermionic determinant $\det D$ is replaced by discretized Brownian noise. This discretization entails step-size errors, so that a delicate and costly extrapolation to zero step-size must be performed. Instead, we use here the multiboson method [5,6]. In its non-hermitian variant, it can simulate 1-flavor QCD [7].

Approximating D^{-1} by a Chebyshev polynomial $P_{2n}(D) = c_{2n} \prod_{k=1}^{n}(D - z_k)(D - \overline{z_k})$, and noticing that $\det(D - \overline{z_k}) = \det\gamma_5(D - \overline{z_k})\gamma_5 = \det(D - z_k)^\dagger$, one obtains

$$\det D \approx \det^{-1} P_{2n}(D) = |\det T_n(D)|^{-2} \qquad (1)$$

with

$$T_n(D) = \sqrt{c_{2n}} \prod_{k=1}^{n} (D - z_k) \qquad (2)$$

The right-hand side of (1) can then be replaced by a Gaussian integral over n bosonic fields ϕ_k. The action is $S_{\text{tot}} = S_{\text{gauge}} + \sum_{k=1}^{n} |(D - z_k)\phi_k|^2$. Because (1) is an approximation, a corrective Metropolis test is added, just like in the 2-flavor algorithm [6]. At the end of each "trajectory" $\{U, \phi\} \to \{U', \phi'\}$, the configuration is accepted with probability $min(1, e^{-\eta^\dagger (W^\dagger W - 1)\eta})$, where $W = [T_m(D')T_n^{-1}(D')][T_m(D)T_n^{-1}(D)]^{-1}$. This algorithm samples the distribution $e^{-S_{\text{gauge}}}\det^{-1}P_{2m}(D)$. With negligible overhead, m can be taken very large ($m \geq 3n$ in our case), so that the measure is effectively $e^{-S_{\text{gauge}}}\det^{-1}P_{\infty}(D)$.

Now the domain of convergence $\mathcal{S}$ of the Chebyshev approximation $P_{2m}(z) \approx 1/z$ in the complex plane is bounded by an ellipse $\partial\mathcal{S}$ centered at $(1,0)$ which goes through the origin. If $z \in \mathcal{S}$, $zP_{2m}(z) = 1 + \mathcal{O}(e^{-\alpha m})$: the approximation is exponentially convergent. Otherwise, $|zP_{2m}(z)| \to \infty$ as $m \to \infty$. This means that configurations for which eigenvalues of D fall outside $\mathcal{S}$ will always be rejected by our algorithm. The measure we sample is $e^{-S_{\text{gauge}}}\det D \ \Theta(\text{spectrum}(D) \in \mathcal{S})$, where $\Theta(u) = 1$ or 0 if u is true or false.

We take for $\partial\mathcal{S}$ a circle, which contains the spectrum of $D = \mathbf{1} - \kappa M$ at $\beta = \infty$ for any $\kappa < \kappa_c = 1/8$, and at $\beta = 0$ for any $\kappa < \kappa_c = 1/4$ in the thermodynamic limit. Thus we expect it to contain the spectrum of D also at intermediate β for $\kappa < \kappa_c(\beta)$, in the thermodynamic limit. Finite-volume fluctuations cause some "exceptional configurations", with eigenvalues outside $\mathcal{S}$, to be included in the exact partition function. Among those are configurations with negative real eigenvalues, for which $\det D < 0$: they create the notorious "sign problem" associated with non-degenerate Wilson quarks. Our algorithm discards such configurations [2].

Therefore, even though it recovers the correct measure in the thermodynamic limit, our algo-

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[2]Note that the R-algorithm would include them in the partition function, but with the wrong sign.

rithm introduces a bias on a finite lattice. This bias however can be viewed as a finite-size effect: it only appears if the inverse quark mass becomes too large compared with the lattice size. For the relatively heavy quarks we consider here, this bias is completely negligible.

The implementation of our algorithm on the Cray-T3D is very similar to the 2-flavor case [6]. Here too, even-odd preconditioning can be implemented through a simple redefinition of the zeroes z_k. Half as many fields ϕ_k are needed for the same quality of the approximation (1). The Metropolis acceptance is shown in Fig.1, to be compared with the 2-flavor case.
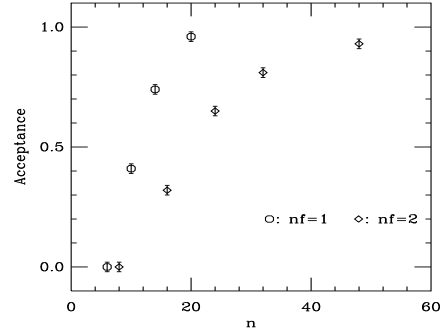

Figure 1. Acceptance versus number of auxiliary fields for $4^4, \beta = 0, k = 0.215$. Circles are $n_f = 1$ data. Diamonds are $n_f = 2$ data.

3. Results

For a fixed κ, we tried to scan β and identify "$\beta_c(\kappa)$". On our rather small lattice, different criteria for criticality will give slightly different effective β_c's. We tried to choose a criterion which reduced finite-size effects, at least in the quenched case. Susceptibility measurements, of the Polyakov loop especially, had large statistical errors and were difficult to exploit. The most useful observables for us were:
i) the histogram of the norm of the Polyakov loop, which shows 2 peaks near criticality. This is safe only if many tunneling events occur between the 2 phases. Fortunately that is the case with our algorithm, as shown in Fig.2 for $\kappa = 0.10$. The work per sweep is roughly equivalent to 6 molecular dynamics steps of the R-algorithm, which

shows that the multiboson approach is rather efficient to decorrelate the Polyakov loop, a global observable.

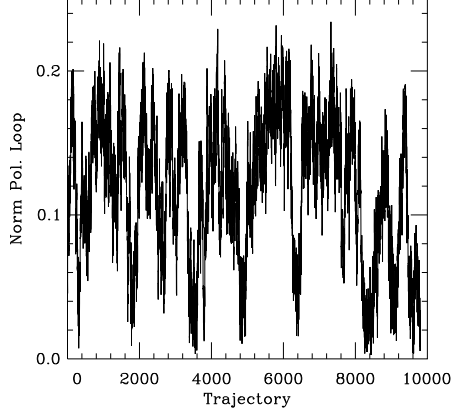ii) the deconfinement ratio $\rho \equiv 3/2p - 1/2$, where

Figure 2. History of the norm of the Polyakov loop for $\beta = 5.67, k = 0.1, L = 8^3 \times 4$. The work per trajectory is equivalent to ~ 6 molecular dynamics *steps*.

p is the probability for the complex trace of the Polyakov loop to fall within $\pm 20°$ of a Z_3 axis. ρ goes from 0 to 1 as the Z_3 symmetry is broken. A preliminary quenched study showed us that identifying β_c as that for which $\rho = 75 - 80\%$ gave very small finite-size corrections.

We then used these 2 observables to determine β_c for $\kappa = 0.05, 0.10, 0.12, 0.14$. The number of auxiliary fields ϕ_k was $8, 16, 24, 32$ respectively. Representative histograms of the norm of the Polyakov loop are shown in Fig.3, to compare with the quenched case. A 2-peak structure remains visible up to the highest κ. One can also clearly see the breaking of the Z_3 symmetry by the dynamical quarks: the peak corresponding to the confined (disordered) phase moves to the right as κ increases. This is evidence for the expected weakening of the phase transition, which should be confirmed by simulations on larger spatial volumes and by finite-size scaling.

Based on Fig.3 and on the measurement of the deconfinement ratio, our estimates for $\beta_c(\kappa)$ are given in Table 1, together with published results for $n_f = 0$ and 2. One sees little departure so far from a linear behavior in n_f: the ordering effect of 1 flavor of quarks is about $1/2$ that of 2 flavors.

κ	N_f	
	1	2
0	5.69254(24)	
0.05	5.685(5)	-
0.10	5.67(1)	-
0.12	5.630(15)	5.58(2)
0.14	5.59(2)	5.46(2)

Table 1: $\beta_c(\kappa)$ for the quenched [8], one- and two-[9] flavor theories

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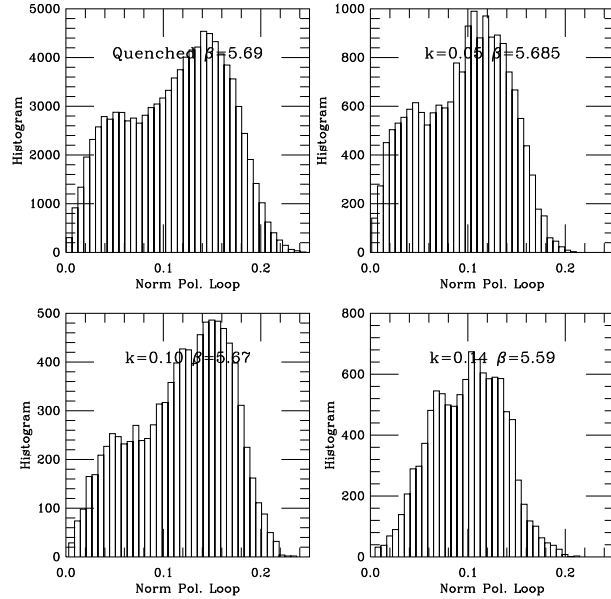9. K.M. Bitar et al., Phys. Rev. D43 (1991) 2396

Figure 3. Histograms of the norm of the Polyakov loop for parameters near β_c.